Contents

Amos RD → Somasundram K, et al. 69
André J-M → Barbier C 363

Barbier C, André J-M: Calculations of molecular polarizabilities using the Valence Effective Hamiltonian (VEH) method 363
Bartha F → Kapny E, et al. 337
Basilevsky MV: The structural stability principle and branching points on multidimensional potential energy surfaces 63
Bertrán J → Ventura ON, et al. 175
Bishop M, Logan D, Michels JPJ: Application of a parallel computer system to polymer calculations 291
Bliznyuk AA → Voityuk AA 223
Bogár F → Kapuy E, et al. 337
Bonaccorsi R → Ventura ON, et al. 175
Bonačić-Koutecký V, Schöffel K, Michl J: Critically heterosymmetric biradicaloid geometries of protonated Schiff bases. Possible consequences for photochemistry and photobiology 459
Brandt BA → Jenč F 411
Brenier B → Rajzmann M, et al. 13

Castro EA → Stradella OG, et al. 57
Ciccarelli L → Garcia E, et al. 253
Čížek J, Vinette F: *N*-dimensional hydrogen atom in an external spherically symmetric field. Symbolic computation and explicit expressions derived from Rayleigh-Schrödinger-type perturbation theory 497
Cremaschi P, Whitten JL: The effect of hydrogen chemisorption on titanium surface bonding 485
Custodio R, Takahata Y: A modification of Koopmans' theorem by imposition of the virial theorem in molecules 197

Dovesi R → Pisani C 277

Edwards WD, Zerner MC: A generalized restricted open-shell Fock operator 347

Faegri K Jr: Energy optimized Gaussian basis sets for the atoms TI-Rn 297
Fantucci P → Gatti C, et al. 433
Filatov MJ, Gritsenko OV, Zhidomirov GM: CNDO-S^2 — a semiempirical SCF MO method for transition metal organometallics 211
Fisher AJ: A comparison of techniques for embedding defect cluster calculations 319

Garcia E, Ciccarelli L, Lagana A: A vectorizable potential energy functional for reactive scattering 253
Gáspár R, Nagy Á: Local-density-functional approximation for exchange-correlation potential. Application of the self-consistent and statistical exchange-correlation parameters to the calculation of the electron binding energies 393
Gatti C, Fantucci P, Pacchioni G: Charge density topological study of bonding in lithium clusters. I. Planar Li_n clusters (n = 4, 5, 6) 433
Ghosh SK, Parr RG: Toward a semiempirical density functional theory of chemical binding 379
Gonoi T → Sasaki F, et al. 123

Grein F, Peyerimhoff SD, Klotz R: Theoretical studies on excited states of Ne_2. III. *Ab initio* spin-orbit studies at large separations for states dissociating to Ne + Ne* (3*s*) 403
Grimley TB: Angle-resolved thermal desorption of atoms from solid surfaces: one-phonon mechanism 475
Gritsenko OV → Filatov MJ, et al. 211

Handy NC → Somasundram K, et al. 69
Handy NC: The Impact of Supercomputers on Chemistry 233
Haug K → Schwenke DW, et al. 237
Hoggan, P, Rinaldi D: Calculation of coulomb integrals in molecules over an *spd* basis of STO 47
Hose G: Multi-reference-state-perturbation theory for computation of potential-energy surfaces 303

Iffert R, Jug K: Treatment of anions in SINDO1 373

Jenč F, Brandt BA: Reduced *ab initio* theoretical internuclear potentials of diatomic molecules 411
Jubert AH → Stradella OG, et al. 57
Jug K → Iffert R 373

Kapuy E, Bartha F, Bogár F, Kozmutza C: Application of the many-body perturbation theory to normal saturated hydrocarbons in the localized representation 337
Klessinger M → Schüle J 35
Klotz R → Grein F, et al. 403
Koga T, Sasaki H: Peculiarity of the Dickinson H_2^+ wave function 27
Kosugi N: Strategies to vectorize conventional SCF-CI algorithms 149
Kouri DJ → Schwenke DW, et al. 237
Kozmutza C → Kapuy E, et al. 337
Krishna Kumar VK, Sen KD: Isoelectronic changes in X-alpha theory using a *Z*-transition state approach 229

Lagana A → Garcia E, et al. 253
Lledós A → Ventura ON, et al. 175
Logan D → Bishop M, et al. 291

Maluendes SA → Stradella OG, et al. 57
Mayer I: On the non-additivity of the basis set superposition error and how to prevent its appearance 207
Michels JPJ → Bishop M, et al. 291
Michl J → Bonačić-Koutecký V, et al. 459
Miller S → Sutcliffle BT, et al. 265
Mota F → Novoa JJ, et al. 325
Murray JS, Politzer P: Electrostatic potentials of some dibenzo-*p*-dioxins in relation to their biological activities 507

Nagy Á → Gáspár R 393
Nomura T → Sasaki F, et al. 123
Noro T → Sasaki F, et al. 123
Novoa JJ, Mota F, Ramirez AC: On the computation of molecular electronic affinities 325

Ohno K → Sasaki F, et al. 123

Osamura Y, Yamaguchi Y, Schaefer III HF: Generalization of analytic energy derivatives for configuration interaction wave functions 71
Osamura Y, Yamaguchi Y, Schaefer III HF: Correspondence between higher order energy derivative formalisms for restricted Hartee — Fock and correlated wavefunctions 93

Pacchioni G → Gatti C, et al. 433
Parr RG → Ghosh SK 379
Peyerimhoff SD → Grein F, et al. 403
Pisani C, Dovesi R: Problems and prospects in the *ab initio* treatment of pure and defective crystals 277
Politzer P → Murray JS 507
Purcell KF → Rajzmann M, et al. 13

Rajzmann M, Brenier B, Purcell KF: Localized virtual and occupied molecular orbitals. Resolution of the difficulties with use of local orbital population as the criterion for localization 13
Ramirez AC → Novoa JJ, et al. 325
Rinaldi D → Hoggan P 47

Sasaki F, Tanaka K, Noro T, Togasi M, Nomura T, Sekiya M, Gonoi T, Ohno K: A data-oriented CI program system 123
Sasaki H → Koga T 27
Savage JR: A parallel architecture and programming language for quantum chemistry 139
Schaefer III HF → Osamura Y, et al. 71, 93
Schöffel K → Bonačić-Koutecký V, et al. 459
Schüle J, Klessinger M: Self-consistent group calculations on a simple model for the photochemical α cleavage reaction of carbonyl compounds 35
Schweitzer, RH → Schwenke DW, et al. 237
Schwenke DW, Truhlar DG: Converged calculations of vibrational energy transfer probabilities for the collision of two HF(v = 1) molecules 1
Schwenke DW, Haug K, Truhlar DG, Schweitzer RH, Zhang JZH, Sun Y, Kouri DJ: Storage management strategies in large-scale quantum dynamics calculations 237
Sekiya M → Sasaki F, et al. 123
Sen KD → Krishna Kumar VK 229
Somasundram K, Amos RD, Handy NC: Disilene, silysilyene and their cations *(Erratum)* 69
Stradella OG, Maluendes SA, Castro EA, Jubert AH: Topological properties of the electronic density of CO-MgF_2 and OC-MgF_2 adducts 57
Sun Y → Schwenke DW, et al. 237
Sutcliffe BT, Tennyson J, Miller S: The use of supercomputers for the variational calculation of rovibrationally excited states of floppy molecules 265

Takahata Y → Custodio R 197
Tanaka K → Sasaki F, et al. 123
Tennyson J → Sutcliffe BT, et al. 265
Togasi M → Sasaki F, et al. 123
Tomasi J → Ventura ON, et al. 175
Truhlar DG → Schwenke DW 1
Truhlar DG → Schwenke DW, et al. 237

Ventura ON, Lledós A, Bonaccorsi R, Bertrán J, Tomasi J: Theoretical study of reaction mechanisms for the ketonization of vinyl alcohol in gas phase and aqueous solution 175
Vinette F → Čížek J 497
Voityuk AA, Bliznyuk AA: MNDO calculations of systems containing hydrogen bonds 223

Whitten JL → Cremaschi P 485

Yamaguchi Y → Osamura Y, et al. 71, 93

Zerner MC → Edwards WD 347
Zhang JZH → Schwenke DW, et al. 237
Zhidomirov GM → Filatov MJ, et al. 211

Indexed in *Current Contents*

Subject index

Ab initio calculations 57
— -Hartree-Fock 277
— LCGO-MO calculations 297
— methods 175
— SCF 507
— — parameters α 393
— statistical parameters α 393
Analytic CI derivatives 71
Analytic energy derivatives 93

Basis set superposition error (BSSE) 207
Bi-electronic integrals 47
Bond electronegativity 379
Bond hardness 379
Branching points 63
BSSE, non-additivity of 207
— , preventing appearance of 207

Charge density topology 433
Charge dependent exponents 373
Chemisorption 485
Close coupling 1
Cluster calculations in solids 319
Collision dynamics 1
Computer memory 237
Correlation energy 337
CPCI equations 71
CI calculation 123
α Cleavage reaction of carbonyl compounds 35
Conventional SCF-CI 149

Data base 123
Defective crystals 277
Desorption 475
Diagonalisation 265
Diatomic molecules 411
Dibenzo-*p*-dioxins 507
Dickinson function 27

Electron affinity 325
— binding energies 393
Electronic structure 379
— structure of metal surfaces 485
Electrostatic potentials 507
Embedding potential 319
Excited state potential energy surfaces 35

File manipulation language 123
Four-index transformation 149

Gaussian basis sets 297
Genealogical data structure 123
Generalized Hartree-Fock theory 347

H_2^+ system 27
Hydrogen adsorption 485
Hydrogen bond 223

Intermolecular interactions 207
I/O bottleneck 149

Keto-enolic tautomerism 175
Koopmans' theorem 197

Lie algebras 497
Linkage CO isomers 57
Lithium clusters 433
Local density approximation 393
— — functional theory 229
Localized orbitals 13, 337

Many-body perturbation theory 337
MBPT-MP2-CIPSI 325
MCSCF and RHF wavefunctions 93
Metallic bond 433
MNDO 47, 223
Molecular anions 373
Molecular electronic structure 123
— linear polarizability 363
Molecules 197
Multireference perturbation theory 303

Negative ions 229

Open-shell Hartree-Fock 347
— molecular orbital theory 347
Overlap population 13

Parallel algorithms 139
— architectures 139
— processing 291
Parametrisation 223
Partition of the ionization energy 197
Perfect crystals 277

Perturbation theory 497
Perturbed hydrogen atom 497
Phonons 475
Photochemical reactions 35
Photoisomerization 459
Pipeline vector computer 1
Point defect theory 319
Polyenes 363
Polymer-Brownian dynamics 291
Potential energy functional 253
— surface calculations 303
— surfaces 63
Potential (internuclear) 411
Program system 123
Protonated Schiff bases 459
Proton transfer 223

Quantum mechanical dynamics calculations 237
Quantum topology 57

Reactive scattering 253
Reduced potential curves 411
Relaxation 197
Restricted Hartree-Fock 347

Scaling 291
Scattering 1
Solvation energy 175
spd basis 47
Spherical tensors 47
Spin-orbit interaction 403
S_0-S_1 conical intersection 459
S^2 terms in CNDO 211
3*s* states of Ne_2 403
Storage management 237
Subdomains of a quantum system 319
Sum-Over-States methodology 363
Supercomputer 253
Supercomputers 237, 265
Supermolecule calculations 207
Symbolic computation 497

Thermal 475
TiH 485
Titanium 485
Transition metal compounds 211
— state method 393

Valence Effective Hamiltonian method 363
Variational method 265
VB−CI 35
Vectorizable canonically-ordered *PK* integrals 149
Vectorization of indirect addressing 149
Vibrational energy transfer 1
Vibration-rotation 265
Vinyl alcohol 175
Virial theorem 197
Virtual orbitals 13
Vision 459

Xα method 393

Zero potential energy 27